

# Quantum phase transitions in bilayer $SU(N)$ anti-ferromagnets

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We present a detailed study of the destruction of  $SU(N)$  magnetic order in square lattice bilayer anti-ferromagnets using unbiased quantum Monte Carlo numerical simulations and field theoretic techniques. We study phase transitions from an  $SU(N)$  Néel state into two distinct quantum disordered “valence-bond” phases: a valence-bond liquid (VBL) with no broken symmetries and a lattice-symmetry breaking valence-bond solid (VBS) state. For finite inter-layer coupling, the cancellation of Berry phases between the layers has dramatic consequences on the two phase transitions: the Néel-VBS transition is first order for all  $N \geq 5$  accessible in our model, whereas the Néel-VBL transition is continuous for  $N = 2$  and first order for  $N \geq 4$ ; for  $N = 3$  the Néel-VBL transition show no signs of first-order behavior.

The study of quantum phase transitions is an exciting field at the forefront of theoretical condensed matter physics [1]. The nature of a particular quantum phase transition is governed by properties that affect long distance physics such as broken symmetries, topological order, the presence of Berry phases and is generally insensitive to microscopic details. Quantum magnets provide the richest examples of quantum phase transitions because they possess internal symmetries in addition to the usual lattice and time reversal symmetries and because they often have non-trivial Berry phases in their long wavelength descriptions [2]. The most popular internal symmetry group in condensed matter is the  $SU(N)$  group. Initial interest was focussed on  $SU(2)$  and the case of  $N > 2$  but finite are interesting in their own right, since they serve to model a number of physical systems ranging from spin-orbit coupled solid-state materials [5] to ultra-cold atoms in optical lattice potentials [6]. While the ground states of  $SU(N)$  spin models in one-dimensional chains are relatively well understood [7, 8], two-dimensional phases [9–11] and their associated phase transitions are only poorly understood.

In this work we address the destruction of the  $SU(N)$  symmetry breaking Néel order in the two-dimensional bilayer system shown in Fig 1(a). In the bilayer geometry the Berry phases cancel between the two layers in the continuum limit allowing access to the phase transitions of interest without the additional complication of quantum interference effects. We have studied the properties of the phase transitions from Néel order to two different types of paramagnetic states, the valence bond liquid (VBL) and the valence bond solid (VBS) [see Fig. 1(b,c)]. The Néel-VBL transition for  $N = 2$  has been studied extensively [12–15] and is well known to be continuous in the  $O(3)$  universality class. Here we address for the first time the fate of this transition when  $N > 2$ . We find that a simple Landau mean-field theory predicts a discontinuous Néel-VBL transition for  $N > 2$  and a continuous transitions for  $N = 2$ . Using unbiased quantum Monte Carlo simulations we confirm the expectations of the Landau theory, except for  $N = 3$ , where we find no evidence for a first-order transition. We show that if this transition is continuous, its

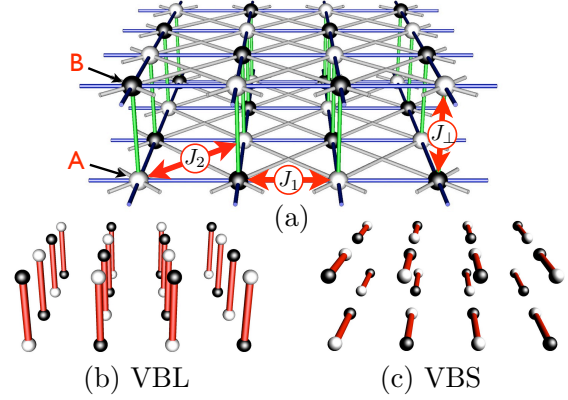


FIG. 1. (a) Bilayer geometry: The white (black) sites are the A(B) sub-lattice on which spins transform as the fundamental (conjugate) representation of  $SU(N)$ .  $J_1$  connects nearest neighbors in the plane,  $J_2$  connect next nearest neighbors in the plane and  $J_\perp$  connect sites on different layers. (b,c) shows cartoon product wavefunctions of local singlets for the VBL and VBS states. In reality, the ground state is a strongly interacting superposition of all valence-bond coverings. The ground state nevertheless (b) preserves all symmetries for the VBL, but (c) breaks lattice-symmetry (as shown) for the VBS. In this paper we provide a detailed study of the Néel-VBL and Néel-VBS quantum phase transitions.

universality class should be identified with a critical point in the compact  $CP^2$  model [16, 17]. The Néel-VBS transition in the single-layer model has been predicted [18] and numerically found to be continuous and in the universality class of the non-compact  $CP^{N-1}$  model for all  $N$  [19–21]. We show that remarkably the Néel-VBS transition characterized by the same broken symmetries becomes first-order in the bilayer geometry for all  $N$  studied here (our model gives us access to  $N \geq 5$ ), a striking consequence of the cancellation of Berry phases between layers.

**Bilayer Model.**— Our  $SU(N)$  symmetric model is defined with a local Hilbert space of  $N$  states on each site of the bilayer square lattice illustrated in Fig. 1(a). We label these states as  $|\alpha\rangle$  with  $1 \leq \alpha \leq N$ . We adopt the representation used previously in both analytic [3, 4, 22] and numerical [21, 23, 24] works on bipartite lattices, where the sublattice-A states transform under rotations with the fundamental repre-

sensation of  $SU(N)$  [generated by the  $N^2 - 1$  matrices  $T^a$ ], and the B sublattice states transform with the conjugate of this representation. We consider two different  $SU(N)$  invariant interaction: between sites  $i$  and  $j$  on the same sub-lattice  $\Pi_{ij} \equiv \sum_a T_i^a \cdot T_j^a$ , and between sites on opposite sub-lattices  $P_{ij} \equiv \sum_a T_i^a \cdot T_j^{*a}$ . Using these interactions, we define a model  $SU(N)$  symmetric bilayer system as follows,

$$H_{\text{bil}} = -\frac{J_1}{N} \sum_{\langle ij \rangle} P_{ij} - \frac{J_2}{N} \sum_{\langle\langle ij \rangle\rangle} \Pi_{ij} - \frac{J_\perp}{N} \sum_{[ij]} P_{ij}, \quad (1)$$

where  $\langle ij \rangle$  denotes nearest neighbors in the square lattice layers,  $\langle\langle ij \rangle\rangle$  denotes next-nearest neighbors in the square lattice layers and  $[ij]$  denotes inter-layer bonds, as illustrated in Fig. 1(a). The  $J_1$  term by itself gives the familiar single layer  $SU(N)$  anti-ferromagnet, which is Néel ordered for  $N \leq 4$  and VBS ordered for  $N \geq 5$ . Adding a  $J_2$  term to the  $J_1$ -model favors the Néel state, causing the Néel-VBS transition to move to arbitrary large  $N$  as  $J_2$  is increased [21]. Finally, when the  $J_\perp$  term is made large enough it always favors the formation of a VBL, by forcing the formation of local singlets [see Fig. 1(b)]. The model bilayer anti-ferromagnet, Eq. (1), reduces to the familiar  $SU(2)$  bilayer model for  $N = 2$  and  $J_2 = 0$ .

Since  $H_{\text{bil}}$  satisfies Marshall's sign criteria, it can be simulated using unbiased quantum Monte Carlo methods on large lattices of linear dimension  $L$  with  $2 \times L \times L$  sites and at finite-temperature  $T$  using the stochastic series expansion method with loop updates [25–27]. Néel order is detected by the existence of a non-zero spin stiffness  $\rho_s = T \langle W^2 \rangle$  in the limit of  $L \rightarrow \infty$ , where  $W$  is the spatial winding number of the world lines [27]. Likewise, long-range order in the correlation function  $N^2 C_V(\mathbf{r}, \tau) = \langle P_{0,0+\mathbf{x}}(0) P_{\mathbf{r},\mathbf{r}+\mathbf{x}}(\tau) \rangle - \langle P_{0,0+\mathbf{x}}(0) \rangle^2$  signals spontaneous translational symmetry breaking, *i.e.*, the onset of VBS order. All the VBS ordering studied in our bilayer system is of the columnar type (at momentum  $(\pi, 0)$ ) and is in phase between the layers (see Fig. 1(c)). We define  $O_{\text{VBS}}^2$  in the usual way as the long distance limit of the VBS correlation function. Finally, an absence of both long-range Néel and VBS orders indicates the formation of a VBL state. Using these tests for the three phases, Néel, VBS and VBL, we have computed the  $T = 0$  phase diagram in the  $g_\perp - g_2$  plane ( $g_\perp \equiv J_\perp/J_1$ ,  $g_2 \equiv J_2/J_1$ ) for each  $N \leq 10$ . For  $N \leq 4$ , the model Eq. (1) has only two phases: Néel and VBL [Fig. 1(b)]. For  $N \geq 5$ , the model admits in addition a VBS phase [Fig. 1(c)]. Phase diagrams for the bilayer model, Eq. (1), for  $SU(2)$ ,  $SU(4)$ ,  $SU(6)$  and  $SU(8)$  symmetry are shown in Fig. 2. These four cases, contain all the types of phase diagrams we have encountered in our study with  $N \leq 10$ . We now turn to the main focus of our paper, a detailed analysis of the nature of the Néel-VBL and Néel-VBS phase transitions that appear in these phase diagrams for each  $N$ .

*Néel-VBL.*— First, we analyze the transition between the Néel state and the featureless fully symmetric valence bond liquid [a cartoon of the VBL state is illustrated in Fig. 1(b)].

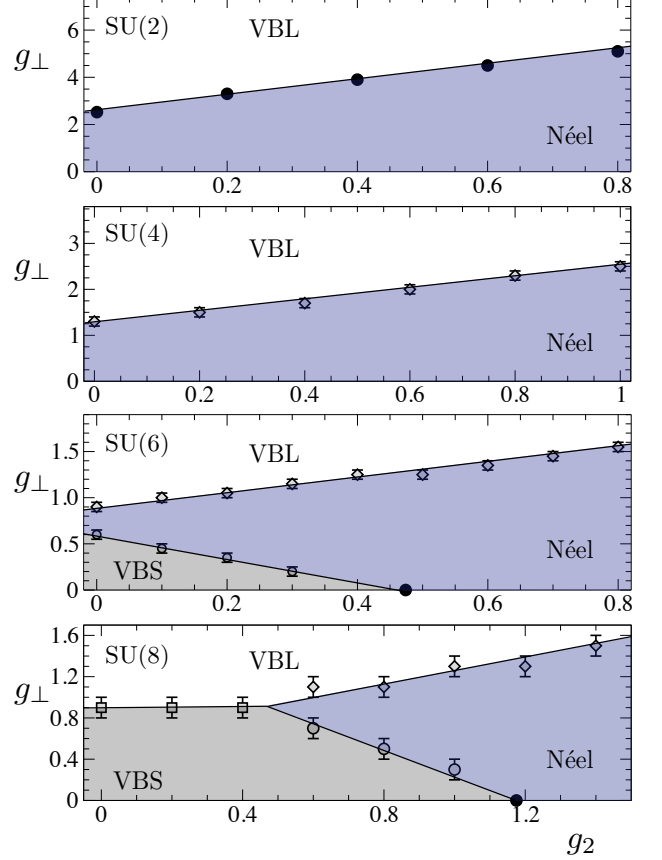


FIG. 2. Phase diagram of the model  $H_{\text{bil}}$  defined in Eq. (1) for  $SU(2)$ ,  $SU(4)$ ,  $SU(6)$  and  $SU(8)$  symmetry in the plane of  $g_2 \equiv J_2/J_1$  and  $g_\perp \equiv J_\perp/J_1$ . The unfilled symbols are locations of first order phase transitions, Néel-VBL (diamonds), Néel-VBS (circles) and VBS-VBL (squares). The solid black circles mark continuous transitions. For  $SU(2)$ , the line of Néel-VBL critical points shown are in the universality class of the  $O(3)$  non-linear  $\sigma$ -model. For  $SU(6)$  and  $SU(8)$  the Néel-VBS transitions shown are in the universality class of the non-compact  $CP^{N-1}$  models (with  $N = 6, 8$  respectively). Solid lines and shaded regions are guides to the eye.

The Néel-VBL transition in the bilayer model for  $N = 2$  and  $J_2 = 0$  has been studied extensively [12–15]. In the special case of  $N = 2$  the order parameter describing the  $SU(2)$  symmetry breaking can be written as an  $O(3)$  vector. The absence of Berry phases in the bilayer geometry then allows for the description of the critical point in terms of the well known  $O(3)$  non-linear  $\sigma$ -model [2]. This simple mapping has no known generalization for  $N > 2$ . For general  $N$ , the simplest description of the Néel-VBL phase transition is found by writing a Landau theory for the order parameter of the  $SU(N)$  anti-ferromagnet. Such a description contains both the Néel and VBL phases, since the VBL is featureless and can be thought of simply as a phase in which the  $SU(N)$  order parameter is quantum disordered. The appropriate order parameter is an  $N \times N$  traceless Hermitian matrix,  $Q_{\alpha\beta}$ , which transforms as

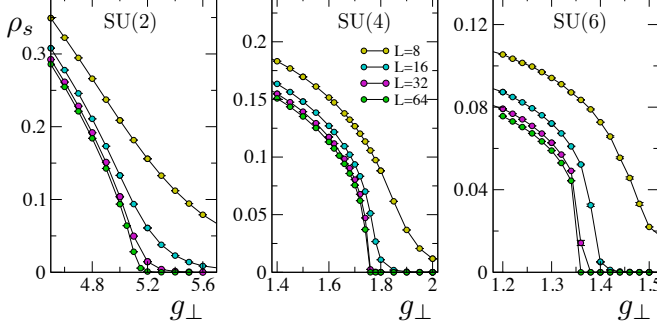


FIG. 3. **Néel-VBL**: The spin stiffness  $\rho_s$  close to the Néel-VBL transition for SU(2), SU(4) and SU(6). The SU(2) transition is continuous and in the O(3) universality class. The quantity  $\rho_s$  for SU(4) and SU(6) show signs of step-like behavior. Close to the step we find double peaked histograms (see Fig. 4) characteristic of a first-order transition. The Néel-VBL transition shows such first order behavior for all  $N \geq 4$ . The parameters used are  $g_2 = 0.8$  for SU(2),  $g_2 = 0.4$  for SU(4) and  $g_2 = 0.6$  for SU(6). The legend shows the value of  $L$ , we have set  $J_1\beta = L$  everywhere.

$Q \rightarrow UQU^\dagger$  under  $SU(N)$  rotation. In our model, Eq. (1), such a matrix can be constructed microscopically from a local operator defined as,  $\hat{Q}_{\alpha\beta}(i) \equiv |\alpha\rangle_i \langle \beta|_i - 1/N$  on the A sub-lattice and  $\hat{Q}_{\alpha\beta}(i) \equiv |\beta\rangle_i \langle \alpha|_i - 1/N$  on the B sub-lattice. We can now coarse grain this local operator to obtain the order parameter,  $\mathbb{Q}$ , and write down a Landau theory action, which being  $SU(N)$  invariant must consist of traces of powers of  $\mathbb{Q}$ .

$$S_L = \alpha_L \text{Tr}(\mathbb{Q}^2) + \beta_L \text{Tr}(\mathbb{Q}^3) + \gamma_L \text{Tr}(\mathbb{Q}^4) \quad (2)$$

Once the order parameter acquires an expectation value we can do an  $SU(N)$  rotation to obtain a diagonal form for  $Q_{\alpha\beta} = m(\delta_{\alpha 1}\delta_{\beta 1} - \delta_{\alpha\beta}/N)$  which is the analog of a “collinear” magnet and the quantity  $m$  is the condensate. If we now substitute the diagonal form for  $\mathbb{Q}$  in  $S_L$  we can see that generally cubic

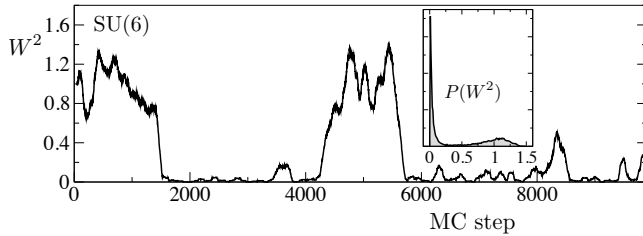


FIG. 4. **Néel-VBL**: Hysteresis and double peaked histograms at a first order Néel-VBL transition in the SU(6) bilayer. In the main frame we show a sample MC history of the binned squared spatial winding number,  $W^2$ , which shows clear evidence for metastability. The inset shows a histogram for the same quantity, with clear double peaked structure. This behavior is found only very close to the transition and for sufficiently large volumes, providing unambiguous evidence for a first order transition. Here shown for  $L = 32$ ,  $g_2 = 0.6$  and  $g_\perp = 1.36$ .

terms in  $m$  are present in the action for  $N > 2$ . In mean-field approach for  $N > 2$  such terms will render the phase transition first order, very much like the first order nematic-isotropic transition in liquid crystals [28]. When  $N = 2$ , it is easy to see that  $\text{Tr}(\mathbb{Q}^3)$  evaluates to zero and does not give rise to a cubic  $m$  term, making a continuous transition possible. Indeed by identifying,  $n_x = (Q_{12} + Q_{21})/2$ ,  $n_y = (Q_{12} - Q_{21})/2i$ ,  $n_z = Q_{11}$  and including gradient terms in the action we arrive at the well known O(3)  $\sigma$ -model for the  $\vec{n} = (n_x, n_y, n_z)$  order parameter.

Consistent with the above Landau theory we confirm from our numerical simulations (see Figs. 3, 4 and 5) that the Néel-VBL phase transition is continuous for  $N = 2$  (and in the O(3) universality class) and first order for  $N \geq 4$ . The first order transitions get progressively weaker as  $N$  is lowered. Indeed for  $N = 3$  we find no evidence for a discontinuous transition up to  $L \leq 128$  [17] (see Fig. 5). If the SU(3) Néel-VBL transition is continuous, what is the continuum field theoretic description? Does the field theory admit a critical fixed point? The continuum description of the Néel-VBL phase transition in our  $SU(N)$  bilayer Hamiltonian is a  $CP^{N-1}$  field theory with a *compact*  $U(1)$  gauge field. In order to make this connection, we introduce  $N$  complex numbers  $z_\alpha$  with the constraint  $\sum_\alpha |z_\alpha|^2 = 1$  [22] and use them to rewrite  $Q_{\alpha\beta} = z_\alpha^* z_\beta - \delta_{\alpha\beta}/N$ . This representation has a well known  $U(1)$  gauge redundancy which can be made explicit with the introduction of a gauge field  $a_\mu$  in the long wavelength effective action, the famous  $CP^{N-1}$  model description,

$$S = \int d^2x d\tau \left[ \frac{1}{g} |(\partial_\mu - ia_\mu)z_\alpha|^2 + F_{\alpha\beta}F_{\alpha\beta} \right] \quad (3)$$

where  $F_{\alpha\beta} = \partial_\alpha a_\beta - \partial_\beta a_\alpha$  is the EM tensor. Following previous work on quantum anti-ferromagnets [29, 30], it is clear that in order for the above field theory to possess the VBL state of the bilayer system when  $J_\perp \gg J_1, J_2$ , the gauge field  $a_\mu$  must be *compact*. The Higgs phase with  $z_\alpha$  condensed corresponds to a phase with  $SU(N)$  symmetry breaking and we identify this phase with the Néel phase. On the other hand, in

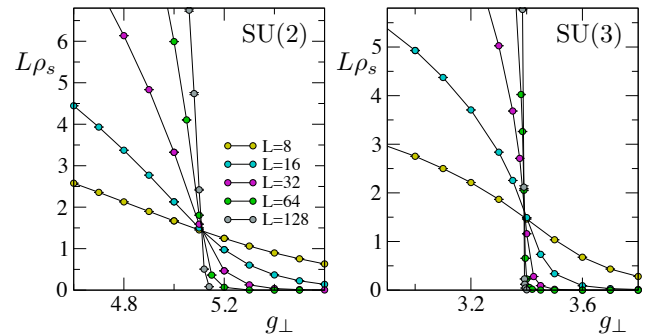


FIG. 5. **Néel-VBL**: Crossings of the fluctuations of the spatial winding number at the Néel-VBL transition for SU(2) and SU(3). In both cases up to sizes of  $L = 128$  we see good evidence for a nice crossing indicating a continuous transition. No evidence for first-order behavior was found in these two cases.

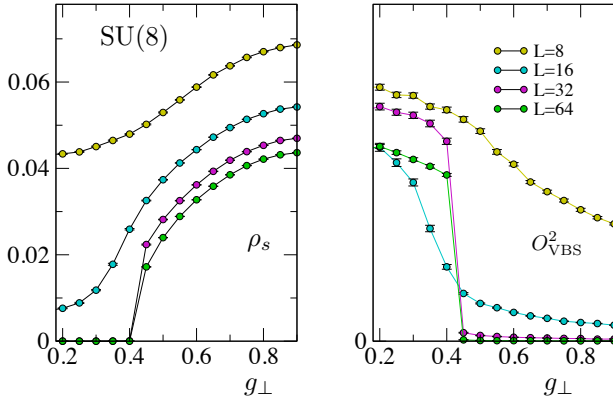


FIG. 6. **Néel-VBS:** First order nature of the Néel-VBS transition in the two dimensional square lattice bilayer. Both  $O^2_{\text{VBS}}$  and  $\rho_s$  show evidence for step like behavior at the same  $g_{\perp}$ . Close to the jump we find the same kind of double peaked behavior in  $\rho_s$  that is illustrated in Fig. 4. Here we have shown sample data for  $N = 8$  and  $g_2 = 0.8$ . Similar behavior is found for all  $N$  studied here.

the phase where  $z_{\alpha}$  is massive, the photon mode gets confined because of the compactness of the gauge field and Polyakov's mechanism of monopole proliferation, resulting in a simple fully gapped paramagnet, which we identify with the VBL phase, Fig. 1(b). Thus the  $SU(N)$  Néel-VBL transition in our bilayer can be described in the continuum limit by the Higgs-“confined phase” transition in the *compact*  $CP^{N-1}$  theory. Recent work [16] has found that a lattice discretization of the compact  $CP^{N-1}$  field theory has a continuous transition for  $N = 2, 3$  and a first order transition for  $N \geq 4$ . Remarkably, this is in full agreement with our findings here for the  $SU(N)$  bilayer, strengthening the evidence for our identification of a continuous transition between Néel and VBL for  $N = 3$ . A detailed study of critical singularities of the  $SU(3)$  Néel-VBL fixed point will be presented elsewhere.

**Néel-VBS.**— We now turn to the transition between the Néel and translational symmetry breaking valence-bond solid state [the VBS state is illustrated in Fig. 1(c)]. For a single layer the Néel-VBS transition in the model defined by Eq. (1) was found to be continuous [21] as predicted by the “deconfined” field theoretic arguments [18]. While it is clear that the Néel and VBS phases are individually stable to a small but finite  $g_{\perp}$ , the interlayer coupling is expected to be strongly relevant at the fixed point of decoupled deconfined quantum critical points. What is the fate of the Néel-VBS transition in the bilayer geometry? From a theoretical point of view, in the bilayer geometry the cancellation of Berry phases negates the quantum interference effects that are crucial to the deconfined quantum criticality scenario [18]. In the absence of such effects one expects the restoration of the conventional Landau paradigm, where the direct transition between two symmetry breaking states is necessarily first-order independent of the value of  $N$ . Indeed as illustrated in Fig. 6 from our QMC simulations we find that the Néel-VBS phase transition is al-

ways first-order in the bilayer geometry. In our model we only have access to this transition for  $N \geq 5$  and in these cases we always find a first-order transition. This is a remarkable effect since the phase transition in the single layer and in the bilayer is in both cases between the same two phases, *i.e.* characterized by exactly the *same sets* of broken symmetries and in the same spatial dimension. The difference in the long-distance physics between the bilayer and single layer, much like the Haldane gap in one-dimension, is purely due to the presence/cancellation of the Berry phases in the single/bilayer systems.

In conclusion we have presented a detailed analysis of two sets of quantum phase transitions in bilayer  $SU(N)$  spin systems: First, we have studied the fate of the popular [12–15] bilayer  $SU(N = 2)$  **Néel-VBL** transition for the case  $N > 2$ , and second, we have studied the fate of the  $SU(N)$  **Néel-VBS** deconfined critical point [18, 21] for a single layer in the bilayer geometry. We have found that the  $N = 2$  continuous Néel-VBL phase transition remains continuous for  $N = 3$  (in the universality class of the compact  $CP^2$  model [16]), becoming first order for  $N \geq 4$ , and that the cancellation of Berry phases in the bilayer geometry restores Landau's paradigm for the Néel-VBS transition, resulting in a first order phase transition between two phases with distinct broken symmetries.

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